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# ATOMISTIC MODELLING OF CROSS SLIP AND ITS CONTRIBUTION TO THE UNDERSTANDING OF TEXTURE AND FATIGUE IN FCC MATERIALS


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# PLAN FOR THE PRESENTATION

- The concept of cross slip
- Atomic-scale modelling of cross slip for copper
- FCC rolling-texture transition
- Fatigue in FCC metals
- Conclusion

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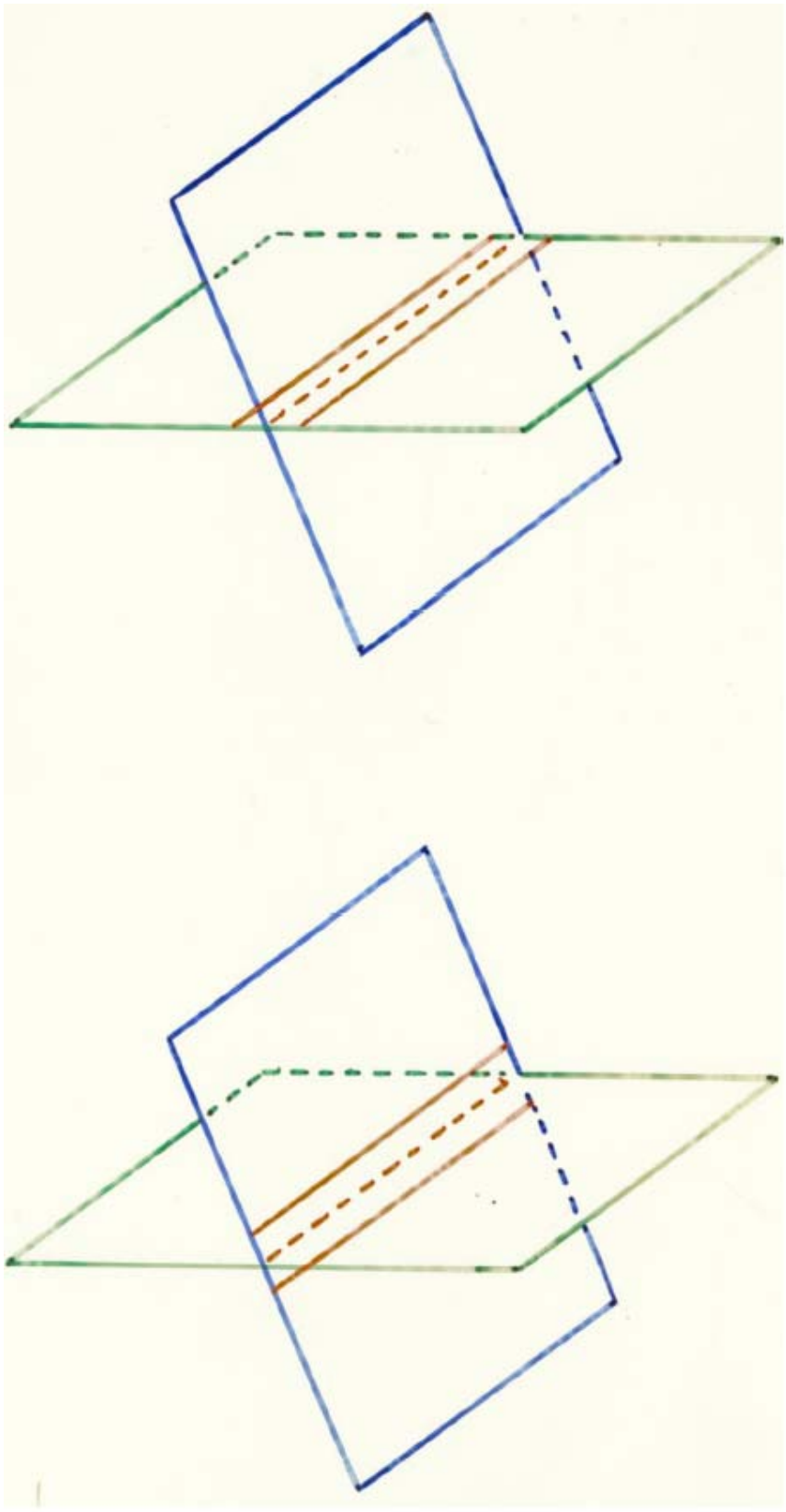
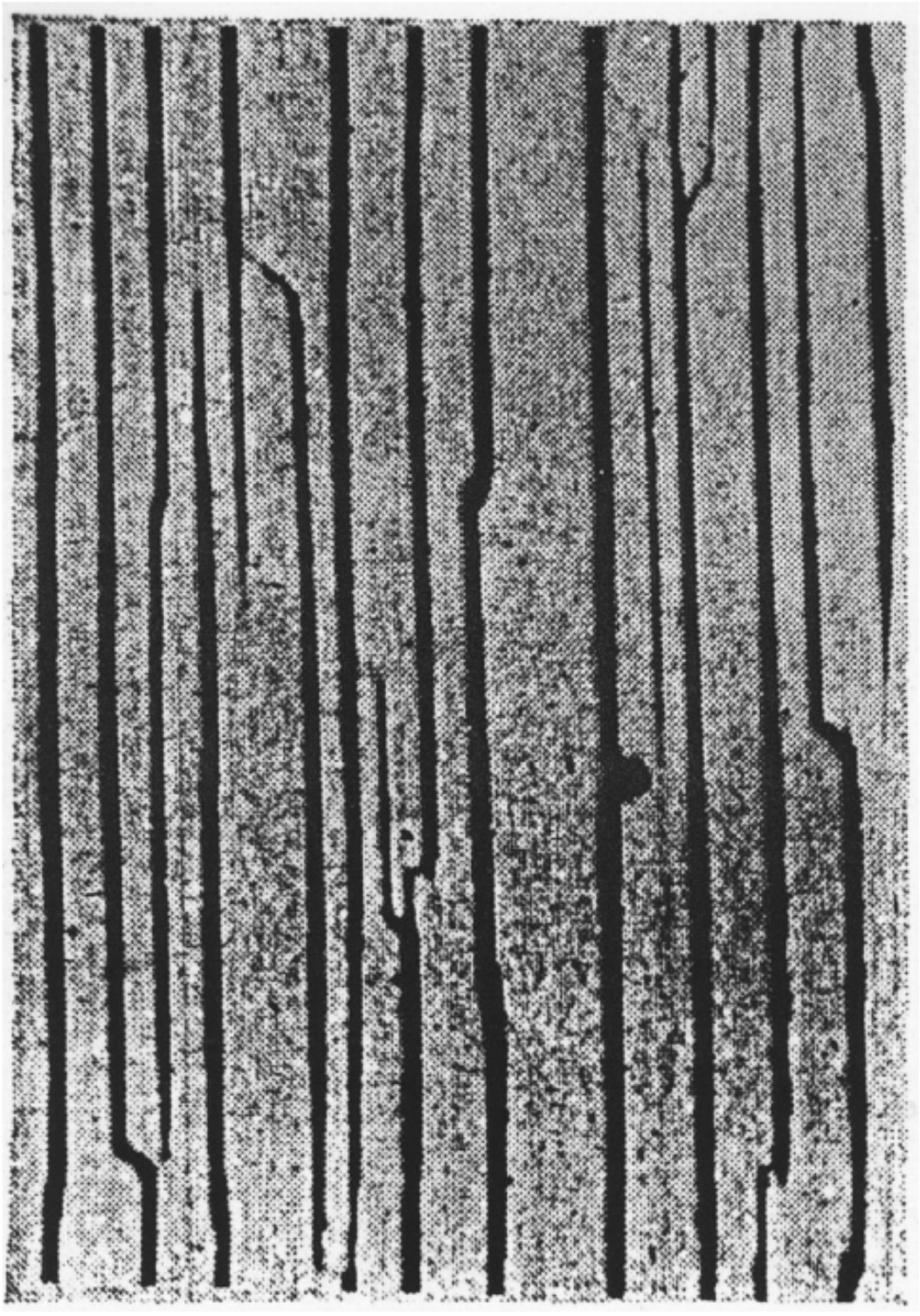
# CROSS SLIP

Normally the slip plane of a dislocation is fixed geometrically. It is the plane defined by the Burgers vector and the line vector.

For screw dislocations Burgers vector and line vector are parallel, and therefore they do not define a specific slip plane.

And therefore screw dislocations can “cross slip”.





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## CROSS SLIP can

- lead to annihilation of screw-dislocation dipoles

- help screw dislocations to bypass obstacles

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# ATOMIC-SCALE MODELLING OF CROSS SLIP

## *Interatomic potential:*

Derived from Effective Medium Theory. The potential reproduces the elastic properties of copper quite well, but it leads to a stacking fault energy of 31 $mJm^{-2}$ which is smaller than the experimentally derived value of ~50 $mJm^{-2}$.

## *Procedure*

Molecular Dynamics is the ideal procedure, but for the typical situation with a complex process like cross slip present-day computers have insufficient capacity for Molecular Dynamics. However, we have succeeded in one case.

Normally we use the "Nudged Elastic Band" procedure. We specify the initial and the final configuration, and the computer finds the minimum-energy pass in multi-dimensional configuration space.

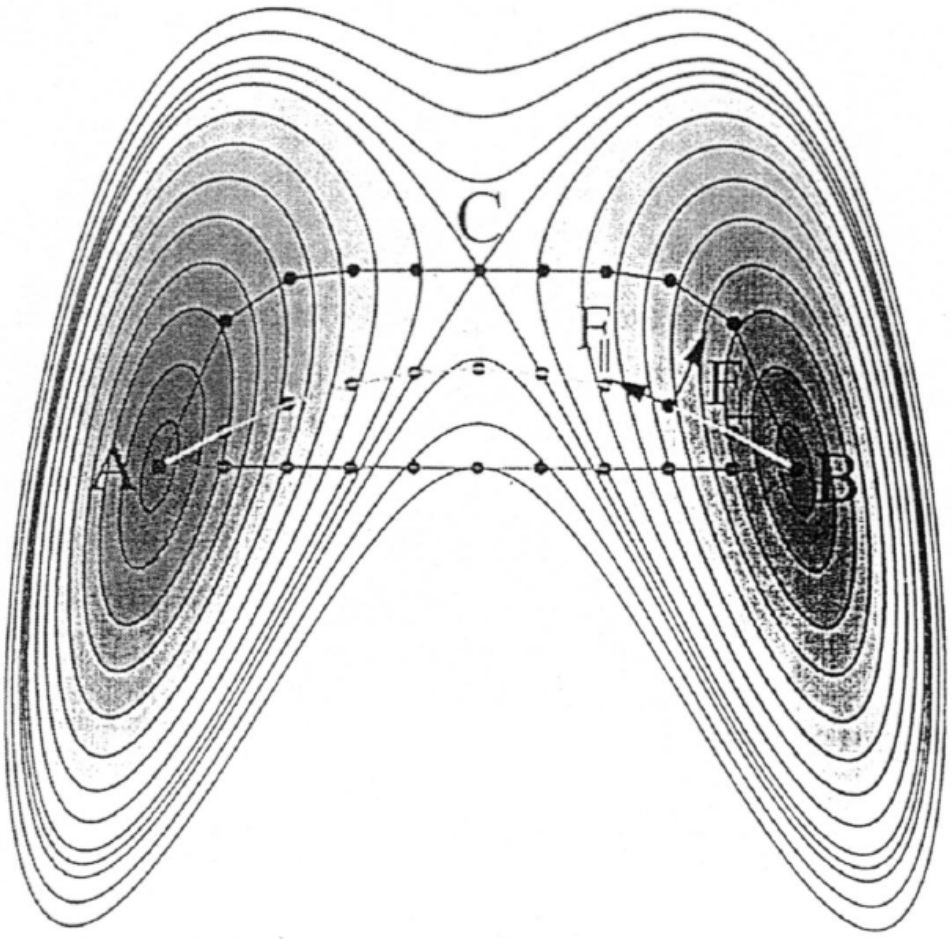


Fig. 1. A schematic representation of a potential energy surface (PES), shown in 2D. The two minima (A) and (B) are separated by a transition state (C). The nudged elastic band (NEB) is used to locate the minimum energy path (MEP), i.e. the path from (A) to (B), where the forces from the potential perpendicular to the path ($F_\perp$) are zero.

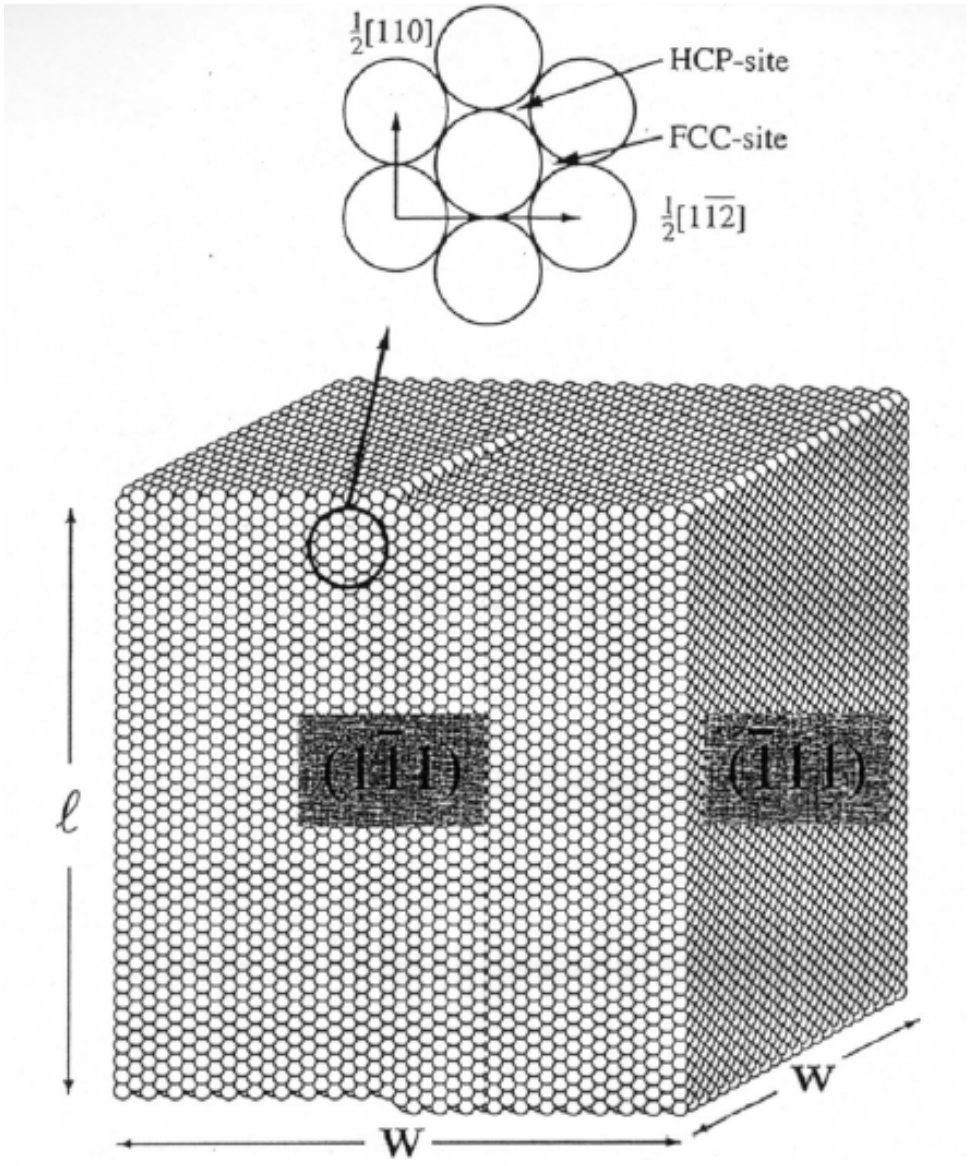


FIG. 2. A medium-size system consisting of 73 960 atoms. The system contains one centered screw dislocation parallel to the [110] direction perpendicular to the top surface. The surface step is parallel to the $(\bar{1}11)$ plane. The width of the two {111} planes is $w=9.5$ nm, and the length of the dislocation (the height of the crystal) is $\ell=40b$ (10.2 nm). The inset shows the difference between fcc and hcp sites in the $(1\bar{1}1)$ plane.

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# RESULTING ACTIVATION ENERGIES

**For an individual non-jogged screw dislocation the theoretical activation energy for cross slip is ~3eV, which is prohibitively high for cross slip at room temperature.**

**For an individual jogged screw dislocation the theoretical activation energy for cross slip is 0.87eV in apparent agreement with the experimental value of 1.15eV ± 0.37eV derived by Bonneville et al. (1988).**

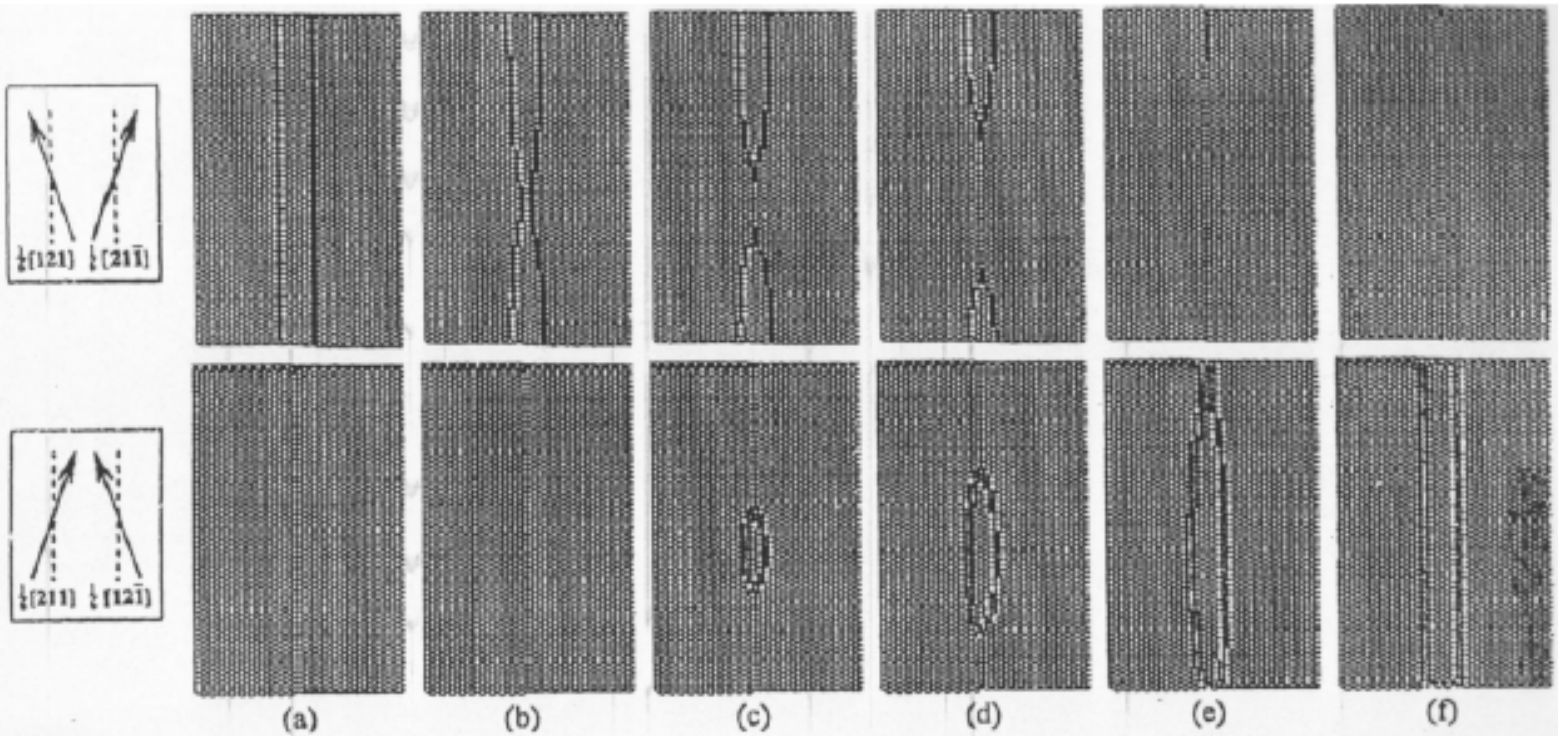
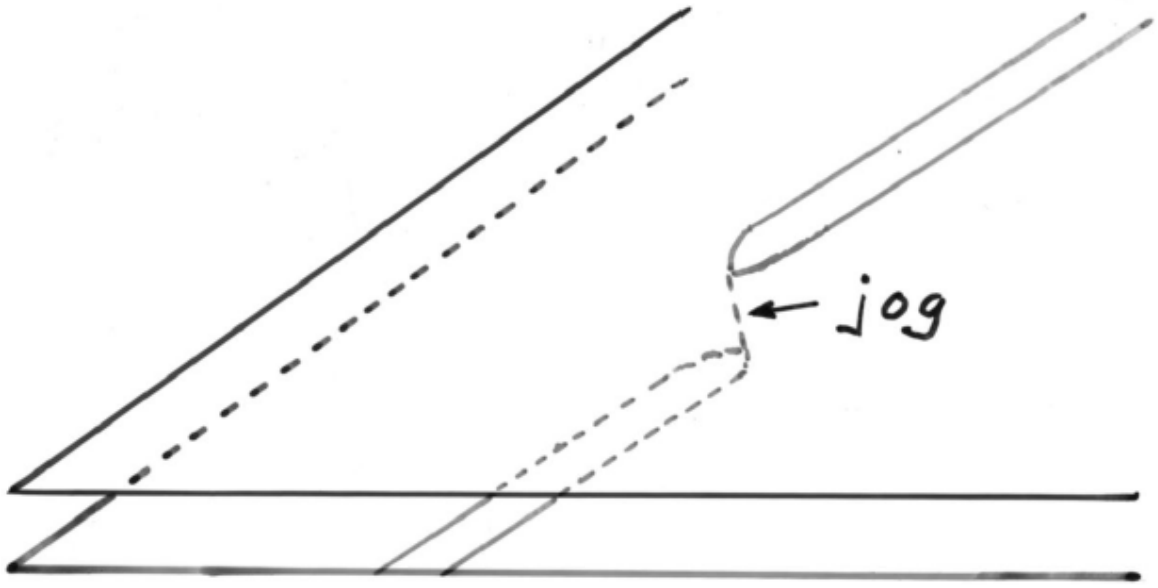



Fig 28. Rasmussen et al. [103]: atomistic calculations according to the nudged elastic band (NEB) method. In the upper row the atom configuration in the primary glide plane, in the lower row the atom configuration in the cross-slip plane is shown. As the dislocation constricts it vanishes from the primary glide plane and emerges in the cross-slip plane.


jog

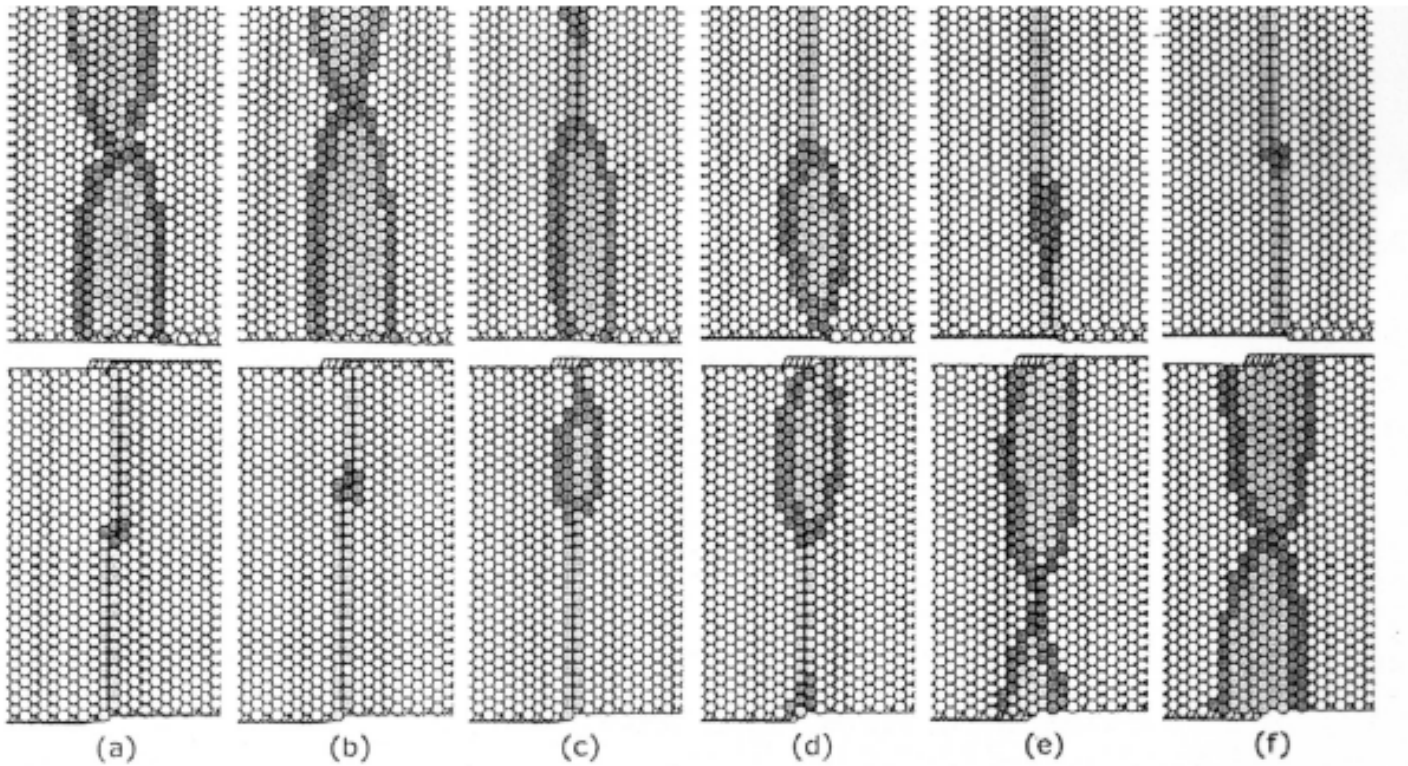



Figure 2. Cross-slip with an elementary jog $\mathbf{l}_2 = a[001]$ moving conservatively in the $(1\bar{1}0)[110]$ non-octahedral slip system, where the top row shows the primary glide plane $(1\bar{1}1)$, and the bottom row shows the cross-slip plane $(\bar{1}11)$: (*a*) initial configuration; (*b*) conservative motion of the jog along the dislocation line; (*c*) unzipping into the cross-slip plane; (*d*) the transition state; (*e*), (*f*) further unzipping into the final config-

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# KINETICS OF CROSS SLIP IN COPPER

## Cross-slip frequency (F) at room temperature

| | E(eV) | F($m^{-3}s^{1}$) |
|---|---|---|
| Without jogs | 3.4 | $4.10^{-25}$ |
| With jogs | 0.86 | $3.10^{16}$ |
| " " " | | |

Time elapsed since Big Bang: $5.10^{17}$s.

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# CROSS SLIP OF ONE ISOLATED NON-JOGGED SCREW DISLOCATION IN "NICKEL"

| | Material | SFE (mJ $m^{-2}$) | E(eV) |
|---|---|---|---|
| Rao et al. | Ni(1) | 58 | 4.85 |
| " " " | Ni(2) | 119 | 2.35 |
| Present authors | "Ni" | 54 | 5.34 |

Rao et al. suggested that their E value of 2.35 eV for Ni(2) can be "translated" to an E value of ~1 eV for Cu – quite different from our E value for Cu of ~3 eV. They ascribe the difference to the different methods.

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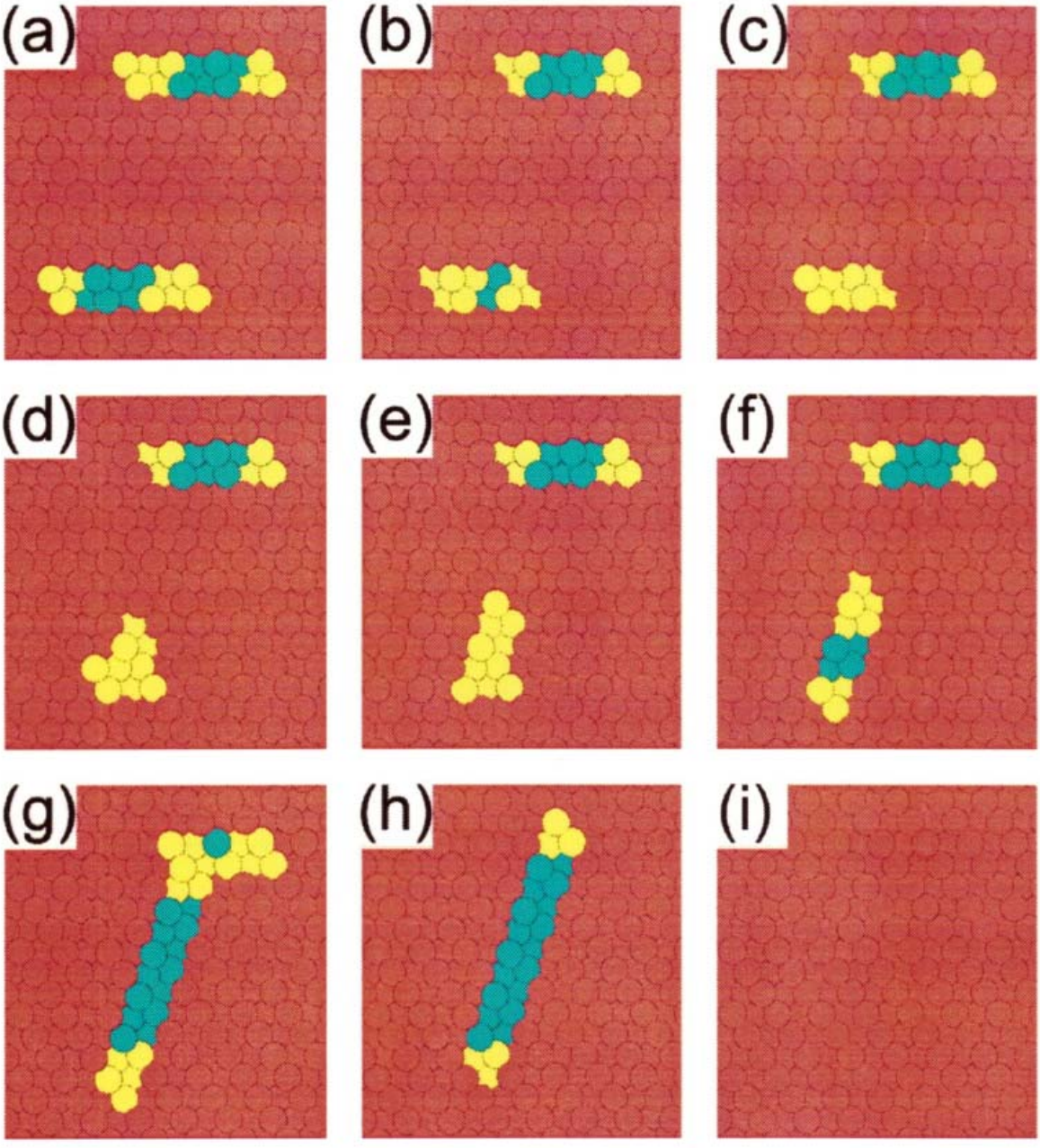
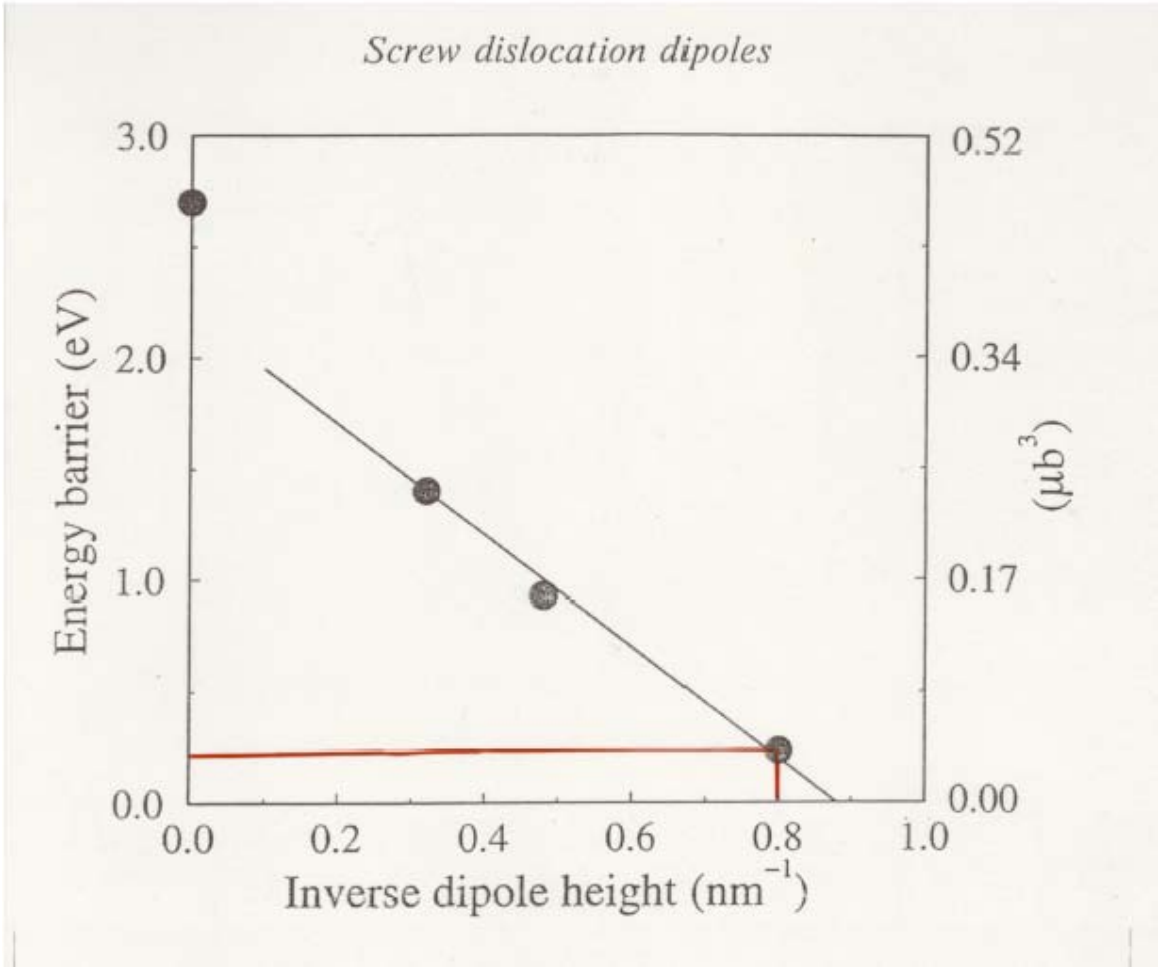
# SCREW-DISLOCATION DIPOLES

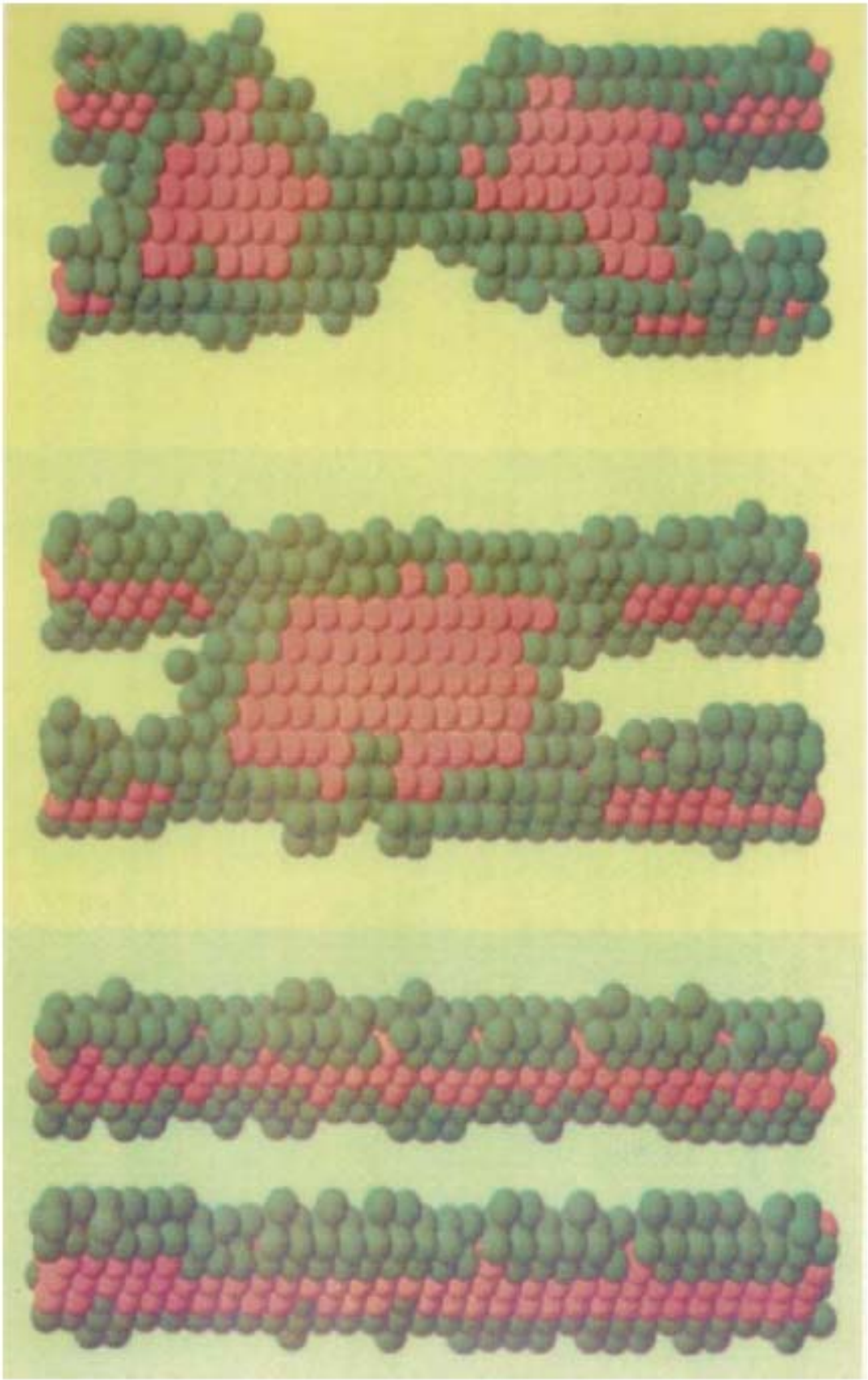
**In screw-dislocation dipoles the attraction between the two dislocations reduces the activation energy for cross slip – the activation energy for dipole annihilation by cross slip.**

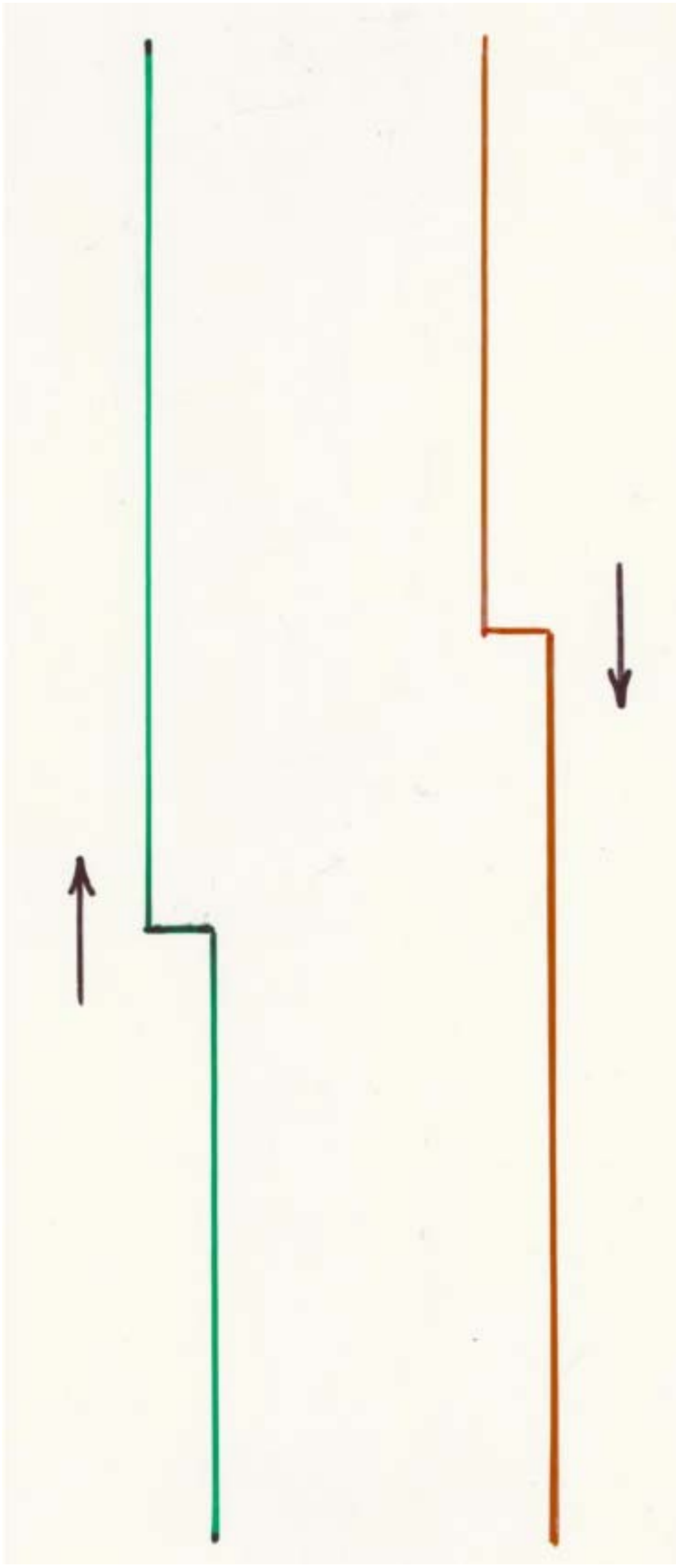
**For non-jogged screw-dislocation dipoles there is a simple reduction of the activation energy with an approximately linear relation between activation energy and inverse dipole height.**

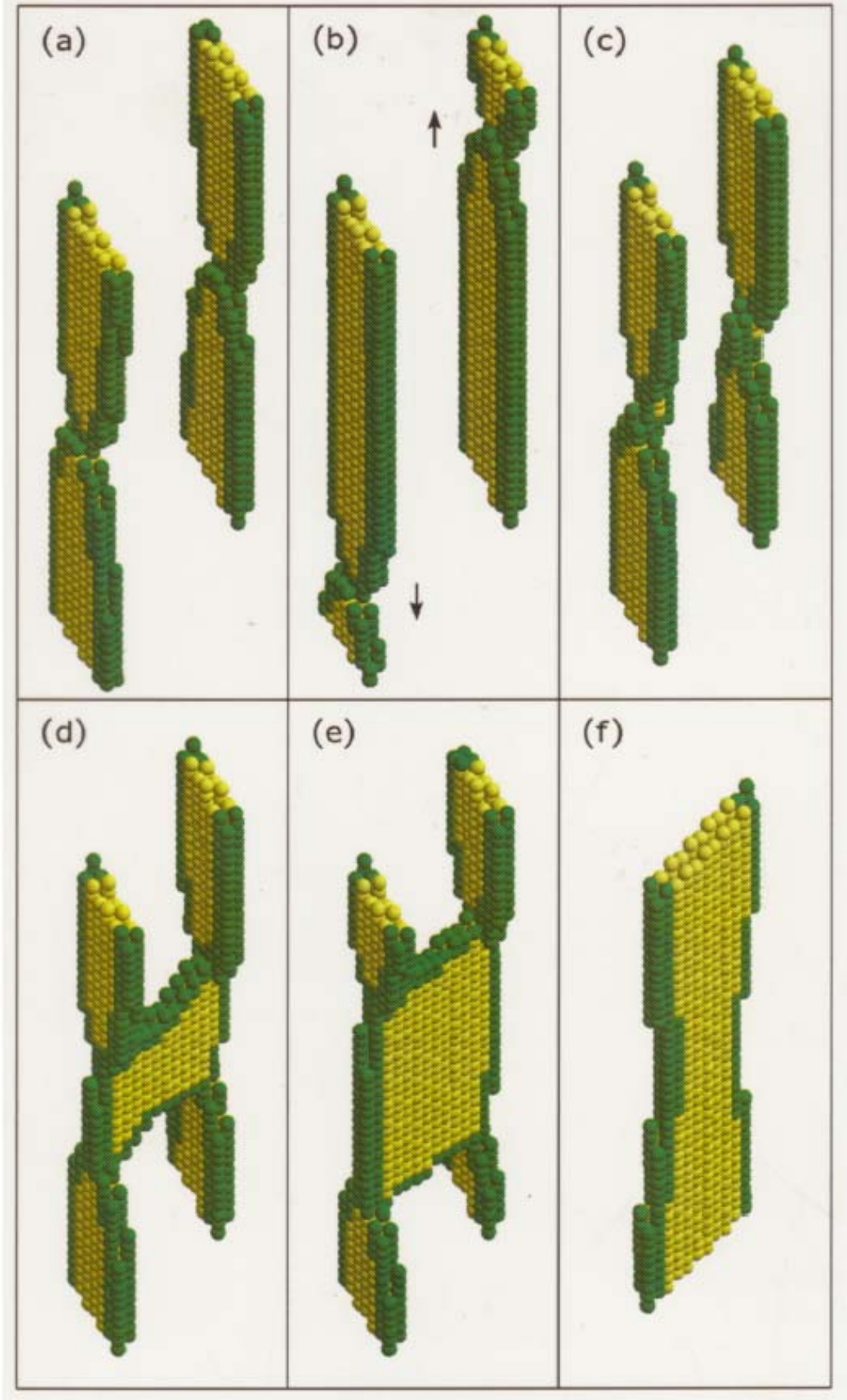
**For jogged screw-dislocation dipoles the computer finds an annihilation mechanism with very low activation energy as an alternative to cross slip: "concerted jog migration". For monotonic deformation we consider concerted jog migration to be an artefact introduced by the periodic-boundary conditions in the computer program. We therefore try to derive the "proper" activation energy for cross slip in jogged screw-dislocation dipoles by enforcing a linear relation with the inverse dipole height.**

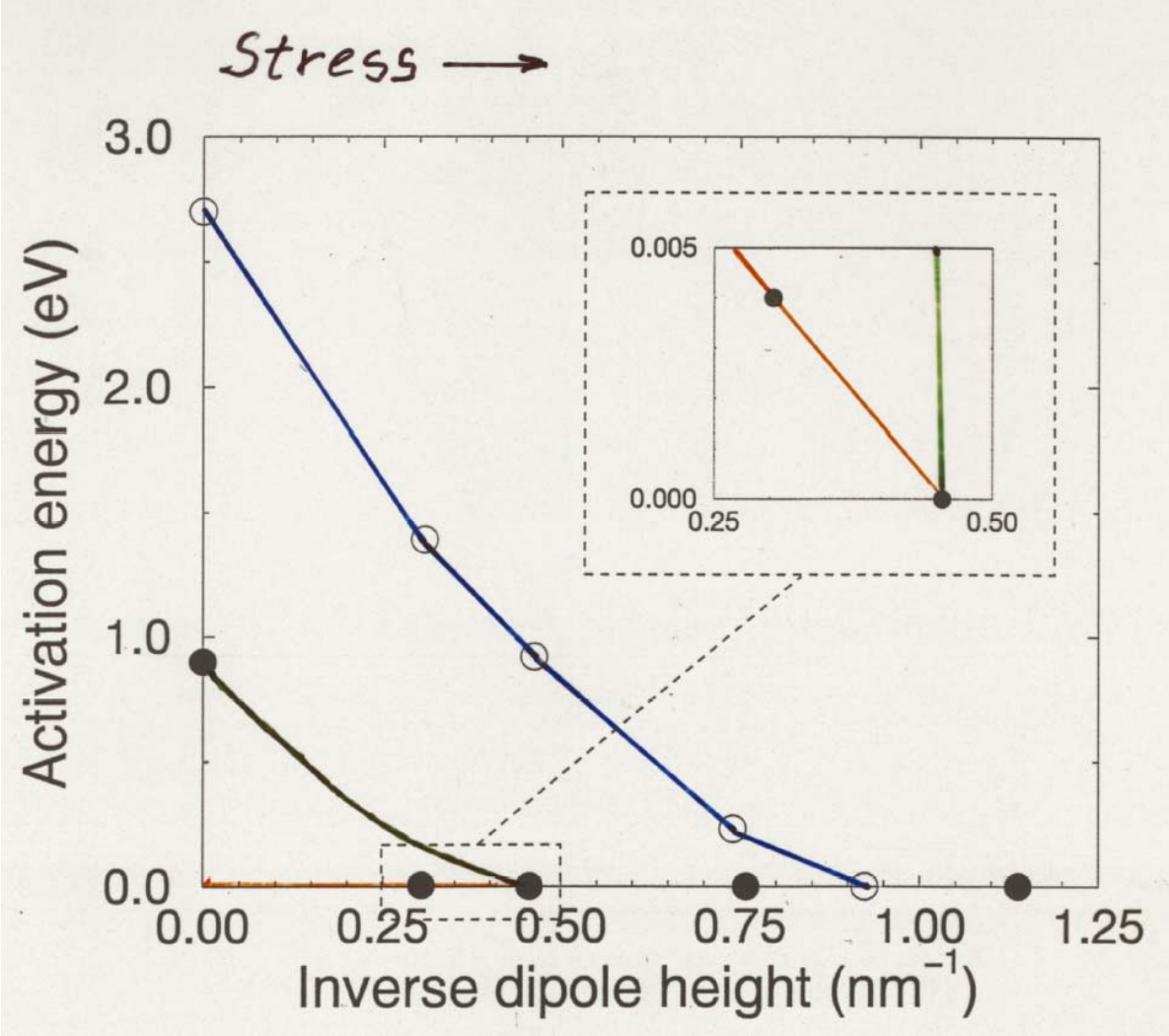

(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
(i)


Screw dislocation dipoles
3.0
2.0
1.0
0.0
Energy barrier (eV)
0.52
0.34
0.17
0.00
(μb^3)
0.0
0.2
0.4
0.6
0.8
1.0
Inverse dipole height (nm^-1)






(a)
(b)
(c)
(d)
(e)
(f)


Stress
3.0
2.0
1.0
0.0
Activation energy (eV)
0.00
0.25
0.50
0.75
1.00
1.25
Inverse dipole height (nm$^{-1}$)
0.005
0.000
0.25
0.50

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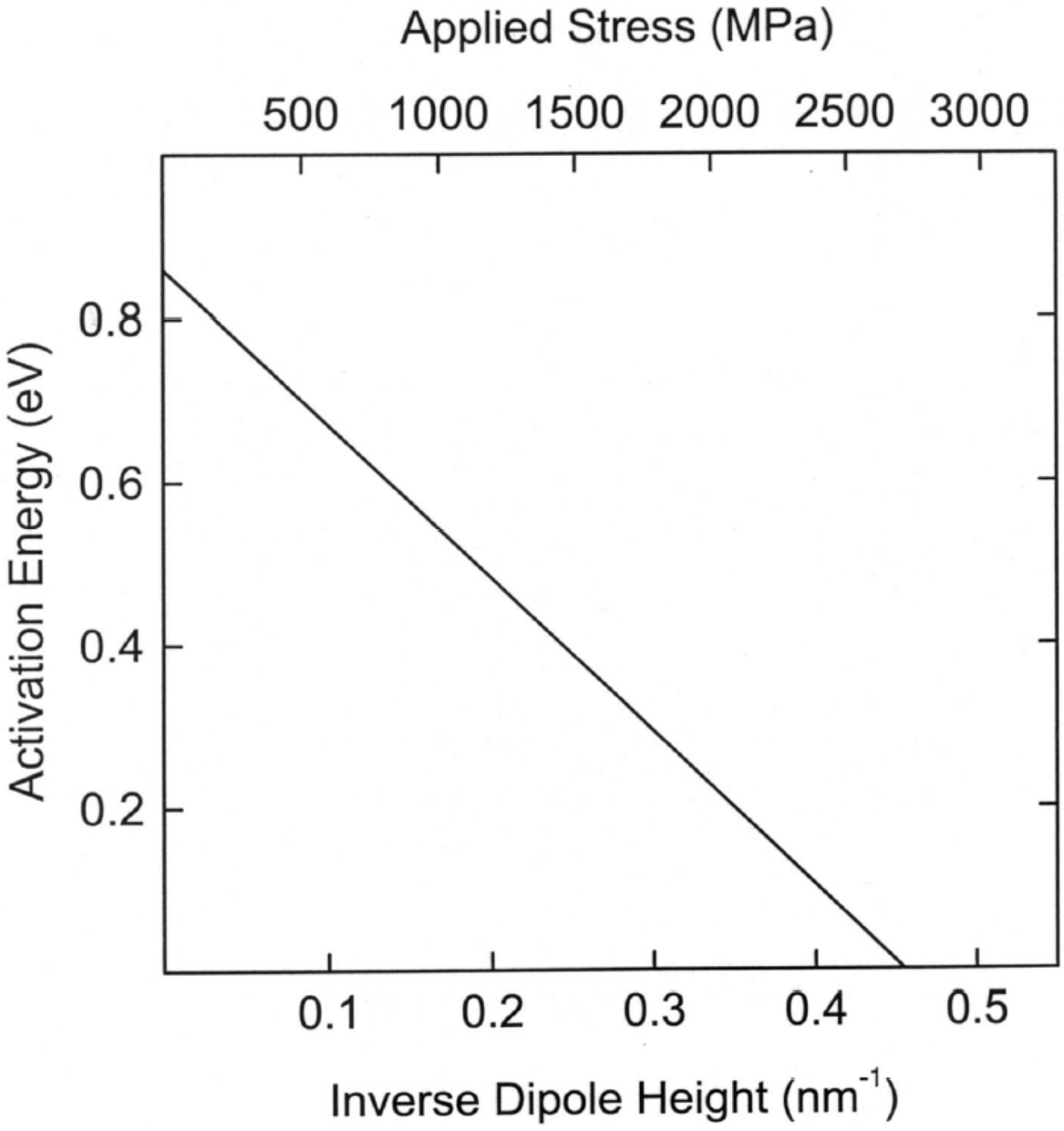
# THE ACTIVATION VOLUME FOR CROSS SLIP

**The activation volume is defined as $dE/d\tau$, i.e. the stress dependence of the activation energy. From the previous figure we derive a theoretical activation volume of ~$10b^3$, *b* being the Burgers vector.**

**The value is much smaller than the experimental activation volume for cross slip in copper as derived by Bonneville et al. (1988) which is ~$250b^3$**

**? ? ?**


Applied Stress (MPa)
500
1000
1500
2000
2500
3000
Activation Energy (eV)
0.8
0.6
0.4
0.2
0.1
0.2
0.3
0.4
0.5
Inverse Dipole Height (nm-1)

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# TEXTURE

**Texture is the statistical representation of the preferred lattice orientations in polycrystals.**

**Texture is an important material parameter. It is the main cause of mechanical anisotropy.**

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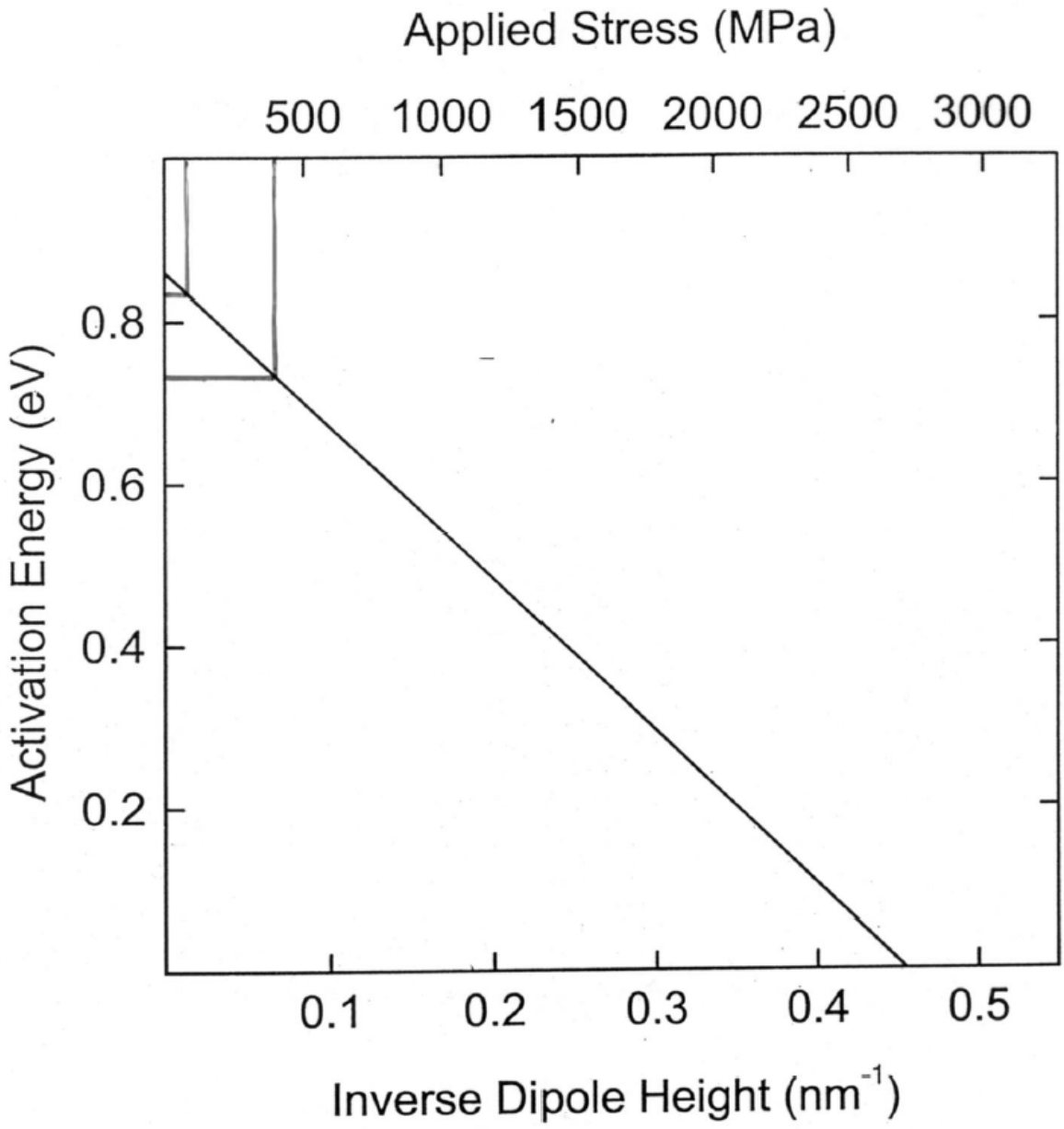
# THE FCC ROLLING-TEXTURE TRANSITION

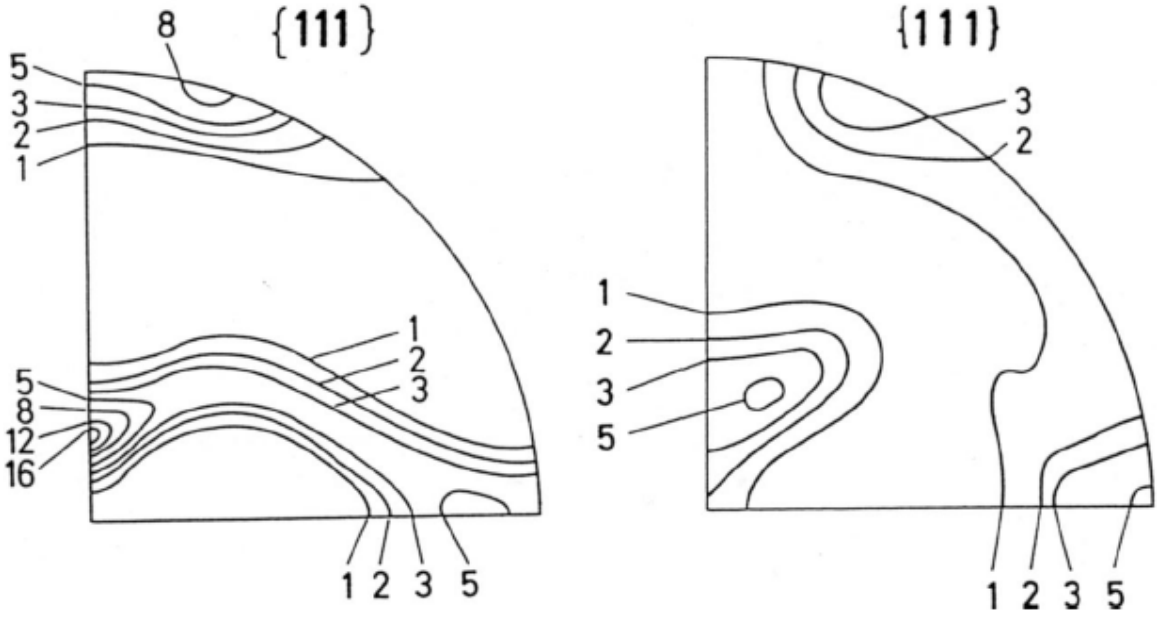
The existence of two types of fcc rolling texture, the copper-type and the brass-type texture, is *the* classical problem in texture research. Already in 1968 Leffers determined the activation energy for the texture transition in Cu-5%Zn by combining the temperature dependence and the strain-rate dependence of the texture after heavy rolling. A recent, revised estimate is **0.70eV±0.10eV**.

The initial flow stress of Cu-5%Zn is ~80MPa, and the flow stress of heavily rolled Cu-5%Zn is ~400MPa which defines a range for the theoretical activation energy for cross slip of **0.83-0.73eV** where the lower value is much closer to the average for the strain range during which the texture is formed than the higher value.

It is an obvious conclusion that the texture transition is governed by cross slip – in accordance with circumstantial evidence.

Notice that the stacking fault energy of "computer copper", 31 $mJm^{-2}$, is close to the actual stacking fault energy of Cu-5%Zn.


Applied Stress (MPa)
500
1000
1500
2000
2500
3000
Activation Energy (eV)
0.8
0.6
0.4
0.2
0.1
0.2
0.3
0.4
0.5
Inverse Dipole Height (nm-1)


{111}
8
5
3
2
1
1
2
3
5
8
12
16
1 2 3 5
{111}
3
2
1
2
3
5
1 2 3 5

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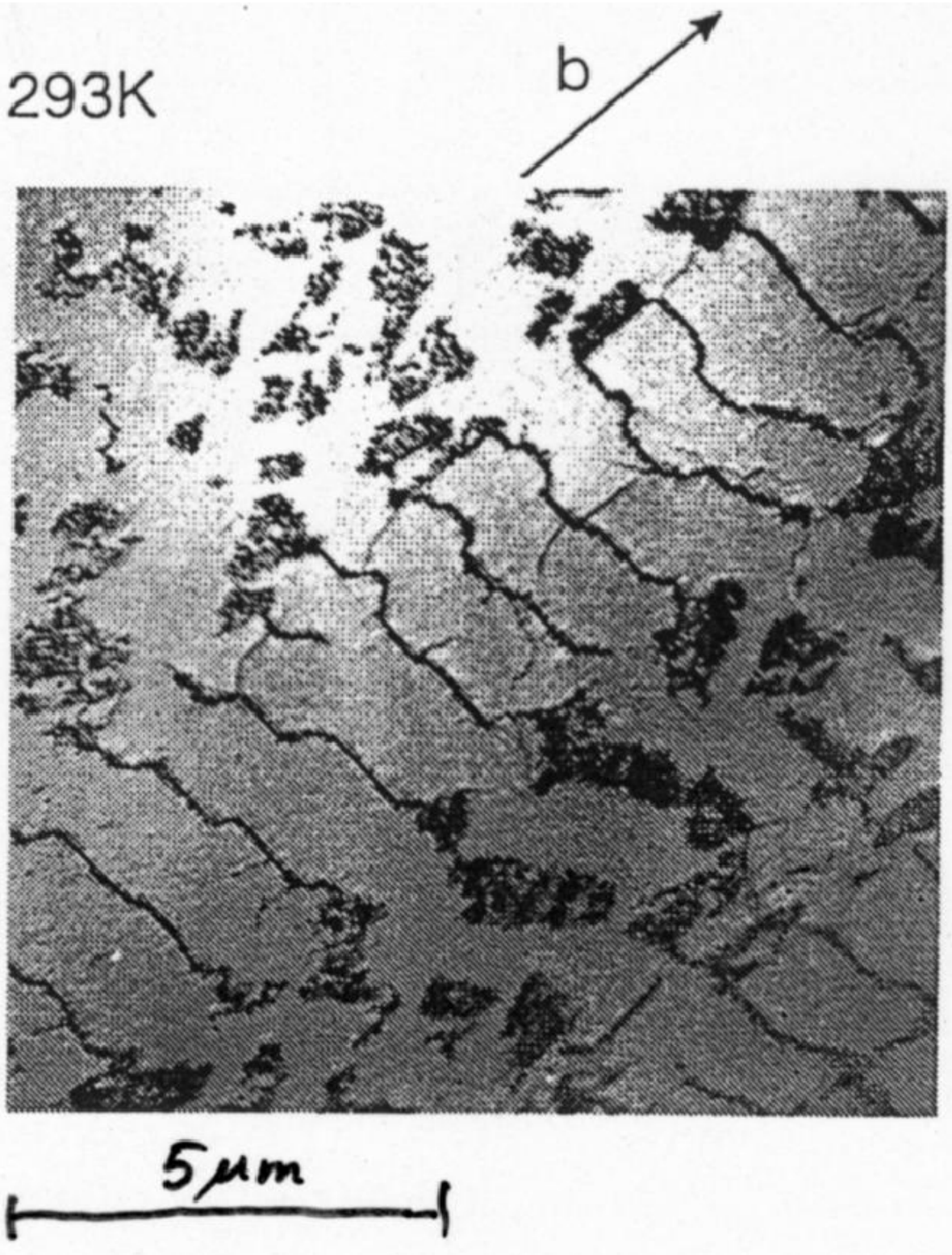
# FATIGUE IN FCC METALS

Cyclic hardening to a saturation stress controlled by persistent slip bands (PSBs) turning into cracks is observed in fcc metals down to 4K. PSBs have a characteristic micro- and nano-structure of thin equidistant edge dipole walls resembling a ladder. In 2000 Pedersen suggested a nanotheory of cyclic saturation, according to which the activation energy for saturation is that for annihilation of unjogged screw dipoles of height $h_{UC}$.


293K
b
5μm

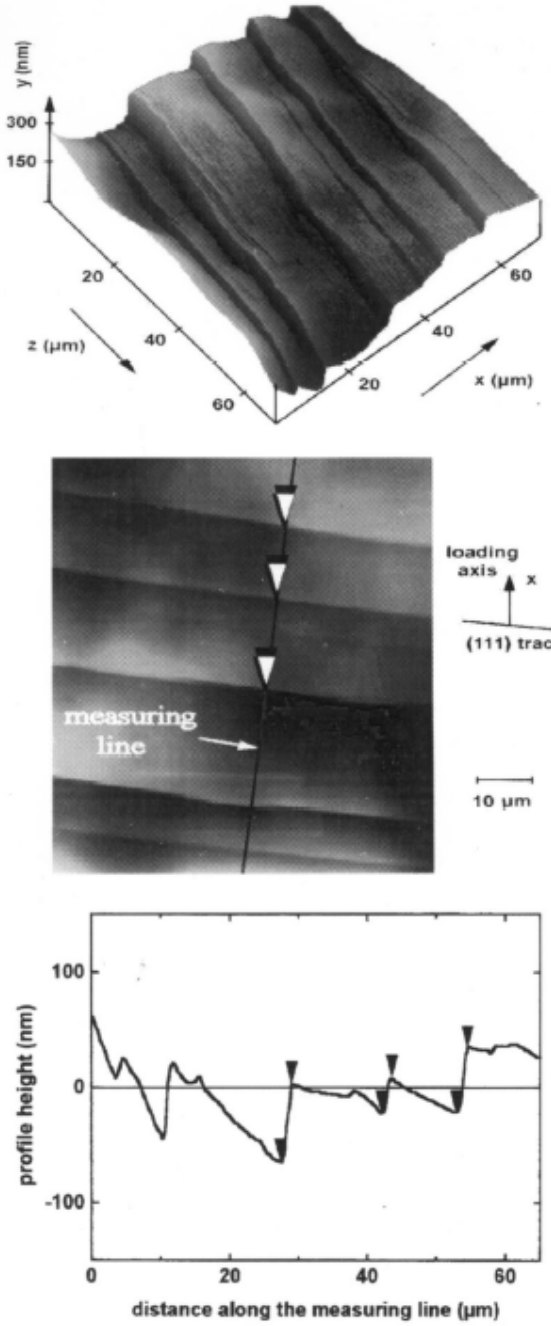



Figure 2. Surface profile developing on the top face of the crystal after one half-cycle tensile plastic strain: (*a*) three-dimensional representation of an AFM image; (*b*), two-dimensional view of the selected area in (*a*) with a measuring line; (*c*) cross-section of the surface profile along the measuring line shown in (*b*).

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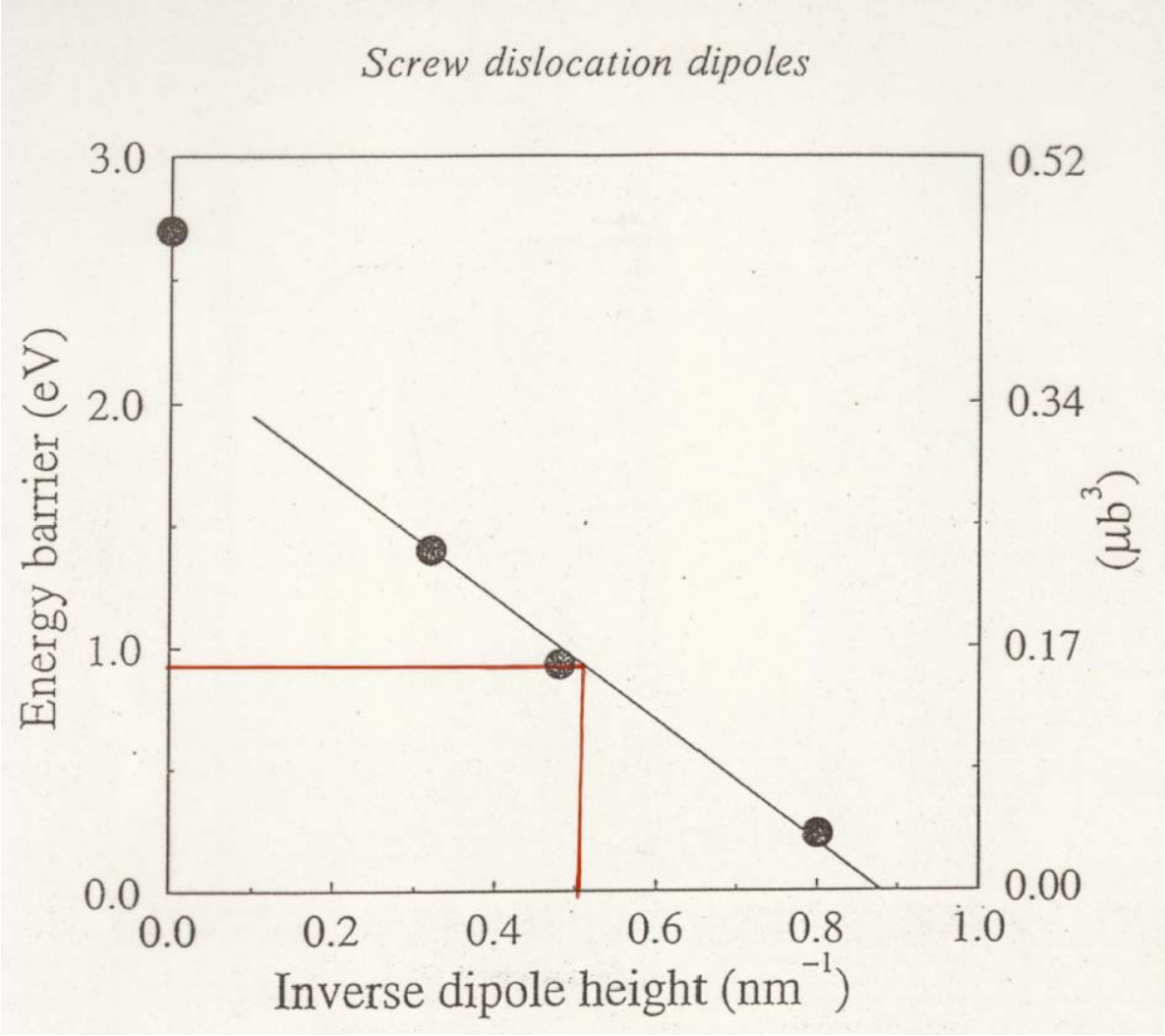
The theory describes cyclic saturation as a thermally activated process of continued nucleation of PSBs deforming heterogeneously by intense plastic shear strain amplitudes $e_{PSL}$ in persistent slip lines (PSLs)

$$e_{PSL} \leq e_{max} = \rho_{ave}(d+w)b+2b/h_{UC}$$

The microstructural parameters $\rho_{ave}$ and d and w can be measured by electron microscoy and $e_{max}$ by methods like atomic force microscopy. For copper fatigued at room temperature this leads to a dipole height $h_{UC}$= 1.7 nm.

The atomistic simulations combined with the activation energy measured from rate- and temperature change experiments lead to a dipole height of $h_{UC}$= 2.0 nm.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0.2
0.4
0.6
0.8
1.0
Inverse dipole height (nm^-1)

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# CONCLUSION

**We have now reached the stage where we can make direct comparisons between the results of atomic-scale modelling and experimental observations. And there seems to be good agreement.**